

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
 Data File : BF102266.D
 Acq On : 20 Jan 2018 15:26
 Operator : SJ/JU
 Sample : J1115-19
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-39-4.0-4.5

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.928	478	483	493	rVB	188791	267778	7.20%	0.828%
2	5.334	547	552	555	rBV	3373694	3586737	96.50%	11.085%
3	6.363	718	727	731	rBV	3214011	3717001	100.00%	11.488%
4	6.493	744	749	752	rBV	3685991	3571406	96.08%	11.038%
5	6.716	784	787	791	rBV	1068338	916068	24.65%	2.831%
6	6.875	810	814	817	rBV	3092190	2768962	74.49%	8.558%
7	7.287	878	884	887	rBV	2202907	2285678	61.49%	7.064%
8	7.387	894	901	907	rBV	60097	83860	2.26%	0.259%
9	7.998	1001	1005	1009	rBV	1294531	1184647	31.87%	3.661%
10	9.081	1183	1189	1192	rBV	3880619	3546748	95.42%	10.961%
11	9.157	1199	1202	1204	rBV	47952	38709	1.04%	0.120%
12	9.475	1251	1256	1258	rBV	495383	454666	12.23%	1.405%
13	9.686	1288	1292	1295	rBV	138419	114603	3.08%	0.354%
14	9.751	1299	1303	1307	rVB	1245565	1164065	31.32%	3.598%
15	10.157	1369	1372	1374	rBV	55446	43134	1.16%	0.133%
16	10.186	1374	1377	1379	rVB	153721	129172	3.48%	0.399%
17	10.404	1408	1414	1416	rBV2	39143	52279	1.41%	0.162%
18	10.545	1431	1438	1441	rBV	1816568	1774433	47.74%	5.484%
19	10.657	1453	1457	1466	rVB	126878	137007	3.69%	0.423%
20	11.104	1530	1533	1536	rBV	84700	74084	1.99%	0.229%
21	11.239	1552	1556	1559	rBV	1040811	950704	25.58%	2.938%
22	11.528	1603	1605	1608	rBV	54537	45524	1.22%	0.141%
23	11.933	1671	1674	1676	rBV2	44777	37445	1.01%	0.116%
24	12.333	1735	1742	1750	rVB4	46951	83546	2.25%	0.258%
25	12.645	1792	1795	1797	rBV	147011	116334	3.13%	0.360%
26	12.822	1821	1825	1828	rBV	2513728	2257380	60.73%	6.977%
27	13.351	1911	1915	1918	rBV	81813	76069	2.05%	0.235%
28	13.716	1973	1977	1985	rBV	344204	359005	9.66%	1.110%
29	13.869	1998	2003	2007	rBV	903554	862524	23.20%	2.666%
30	14.039	2028	2032	2035	rBV2	39191	37879	1.02%	0.117%
31	14.345	2080	2084	2091	rVB2	145056	160701	4.32%	0.497%
32	14.957	2185	2188	2192	rBV	221066	245456	6.60%	0.759%
33	15.292	2240	2245	2249	rBV	645932	773705	20.82%	2.391%
34	15.510	2278	2282	2293	rVB4	49658	77691	2.09%	0.240%

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ALS Vial : 16 Sample Multiplier: 1

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ClientSampleId :
SB-39-4.0-4.5

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	15.727	2314	2319	2323	rBV2	50841	84224	2.27%	0.260%
36	15.774	2324	2327	2334	rVB4	45068	68072	1.83%	0.210%
37	16.480	2441	2447	2453	rVB2	119363	209255	5.63%	0.647%

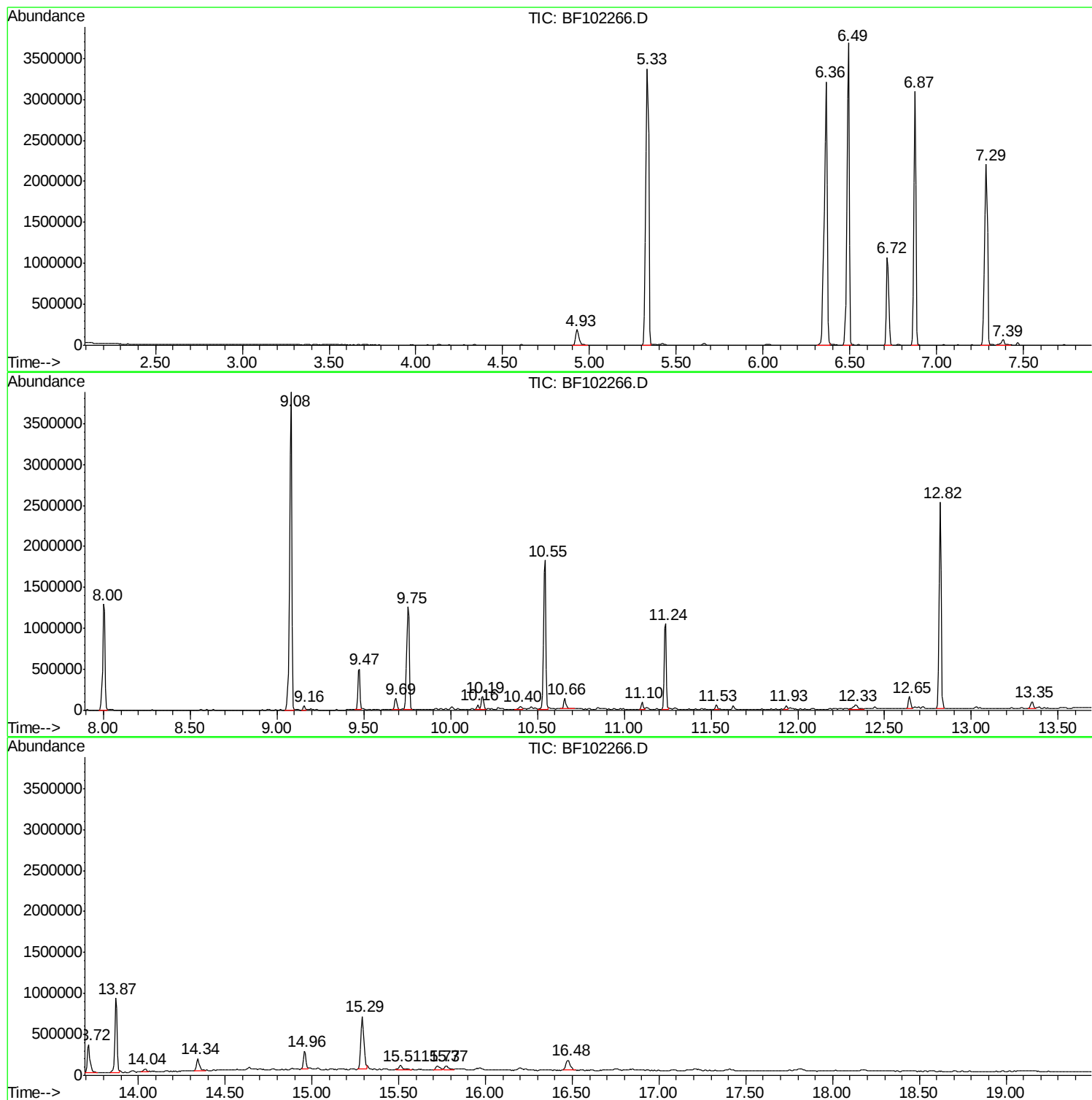
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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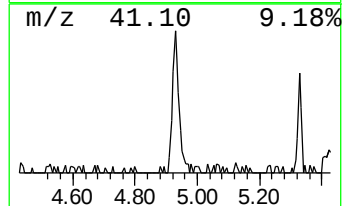
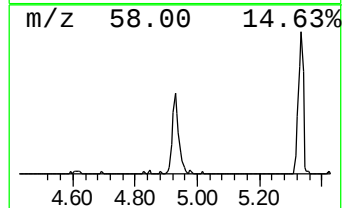
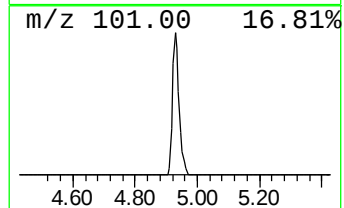
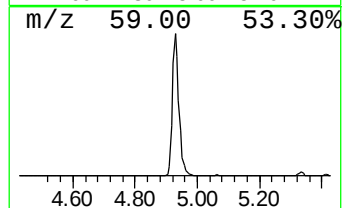
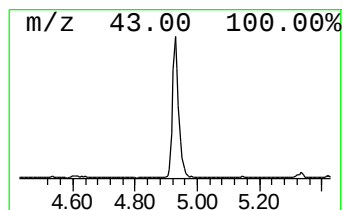
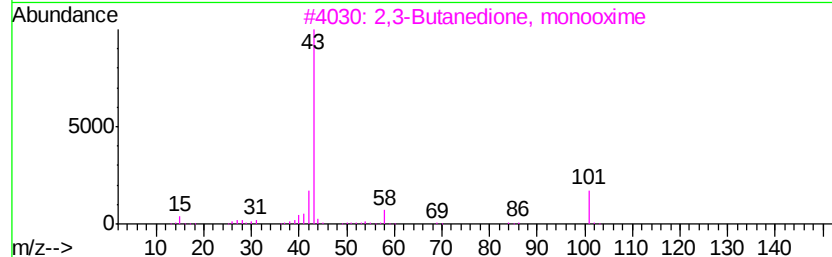
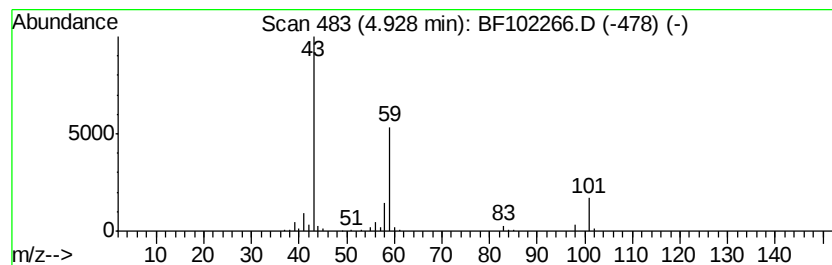
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	5.85 ng	267778	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	Butane	58	C4H10	000106-97-8	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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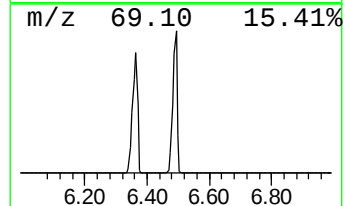
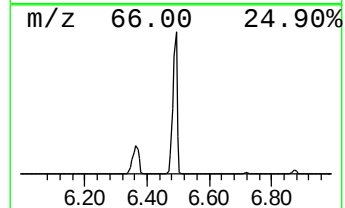
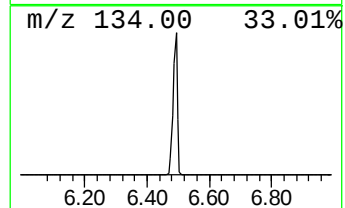
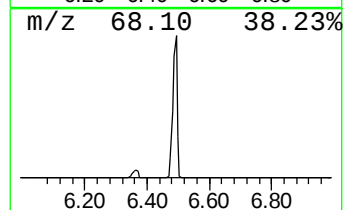
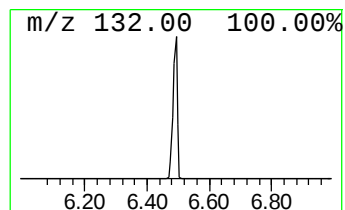
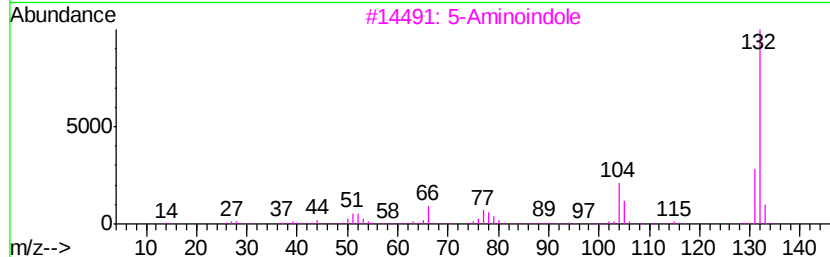
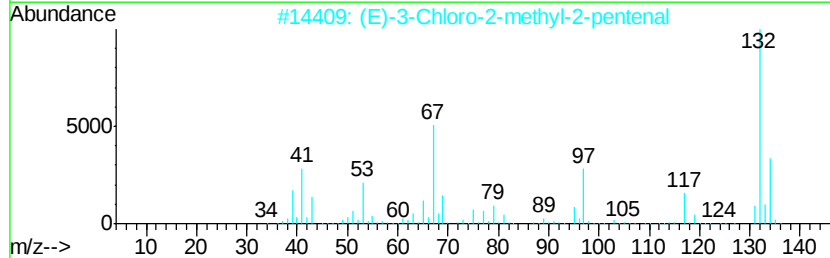
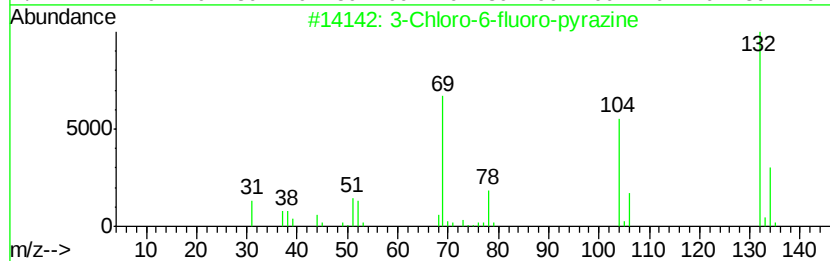
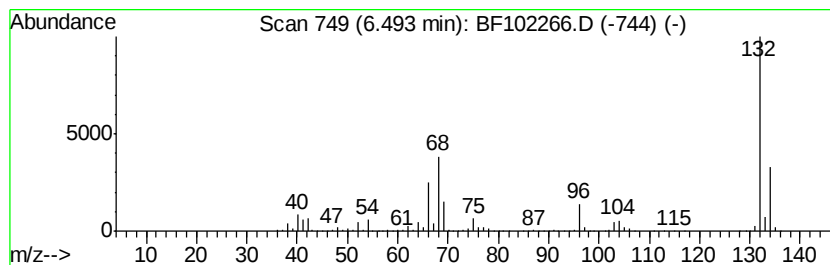
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	77.97 ng	3571410	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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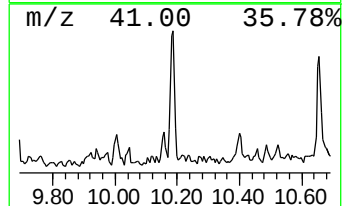
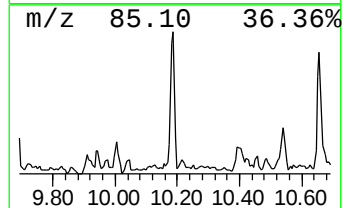
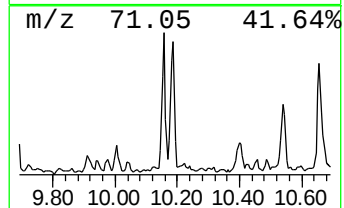
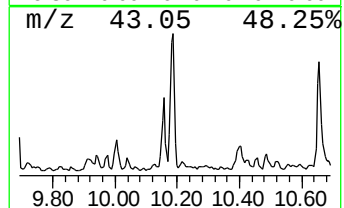
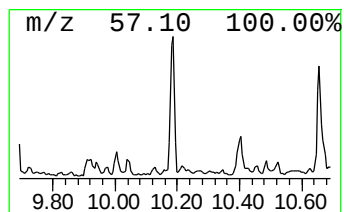
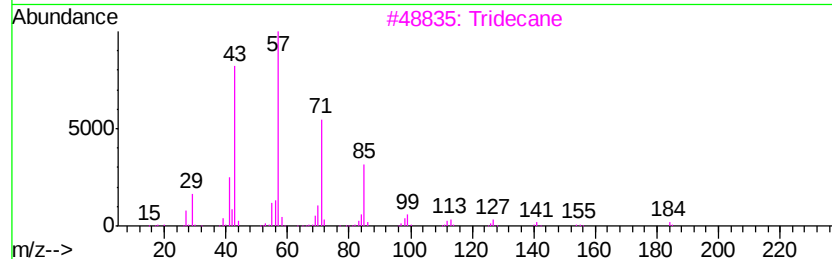
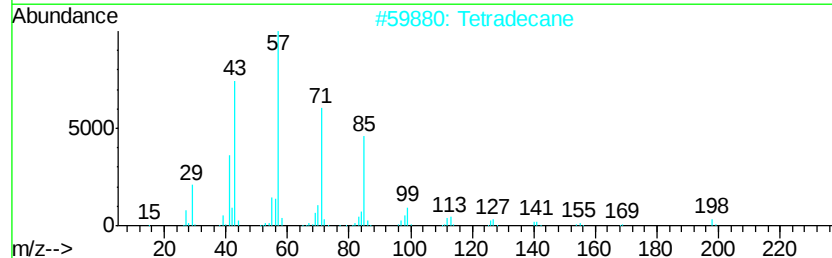
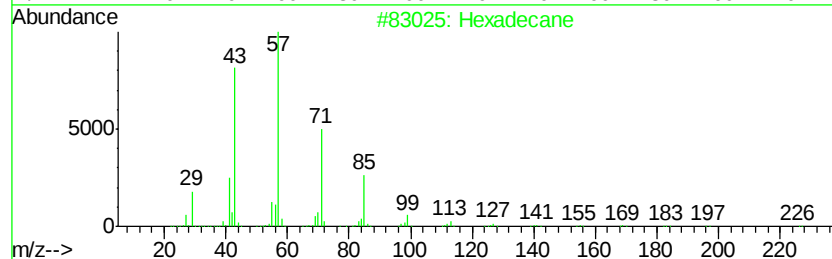
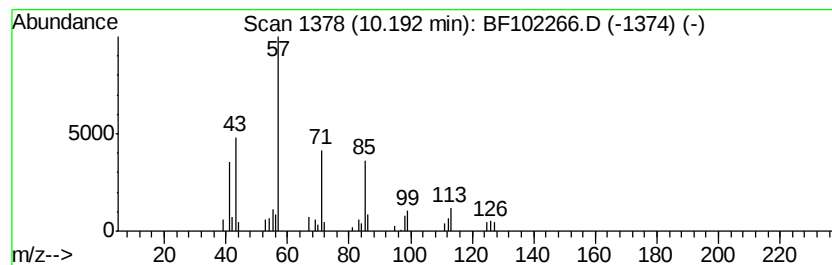
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.19	2.22 ng	129172	Acenaphthene-d10	9.75
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	90
2	Tetradecane	198 C14H30	000629-59-4	80
3	Tridecane	184 C13H28	000629-50-5	78
4	Octadecane	254 C18H38	000593-45-3	64
5	Tetradecane, 1-iodo-	324 C14H29I	019218-94-1	59



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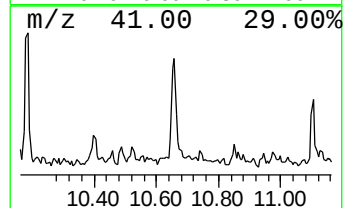
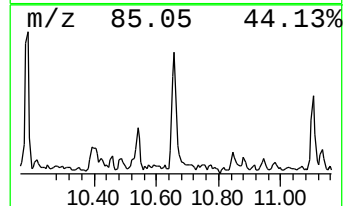
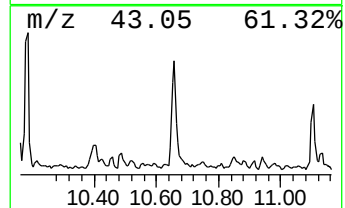
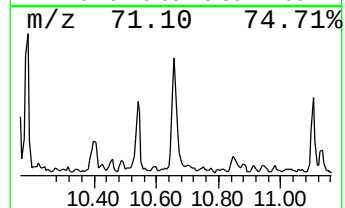
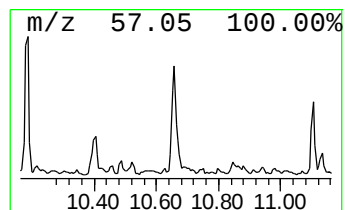
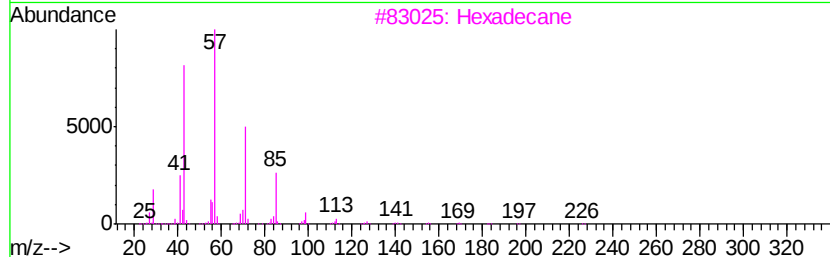
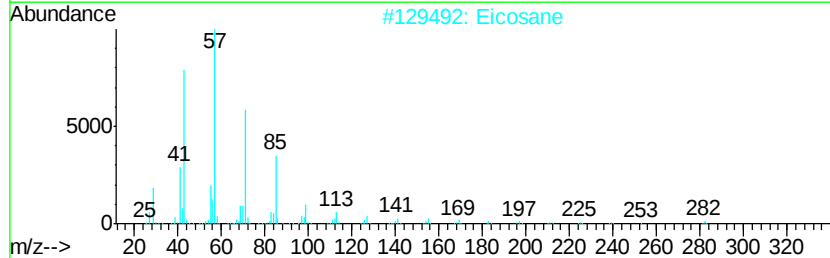
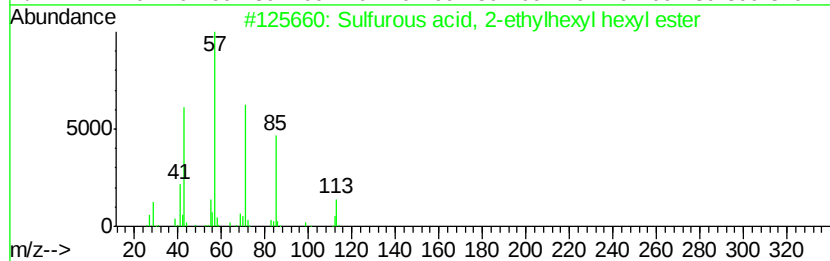
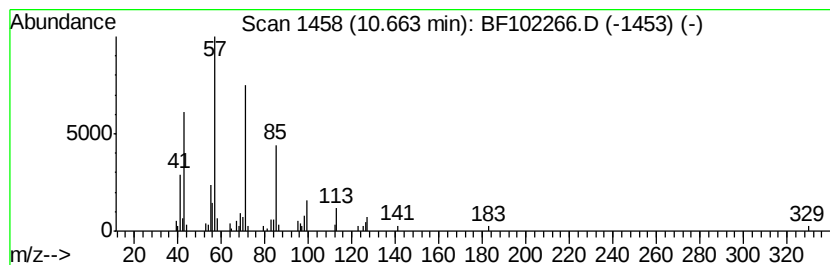
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Sulfurous acid, 2-ethylhexy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.88 ng	137007	Phenanthrene-d10	11.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	86
2		Eicosane	282	C20H42	000112-95-8	86
3		Hexadecane	226	C16H34	000544-76-3	83
4		Tetradecane	198	C14H30	000629-59-4	83
5		Tetracosane	338	C24H50	000646-31-1	78



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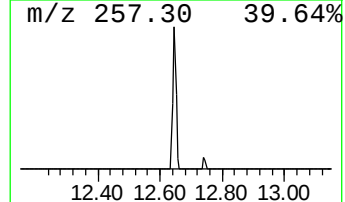
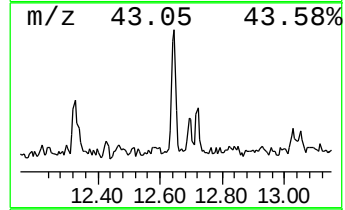
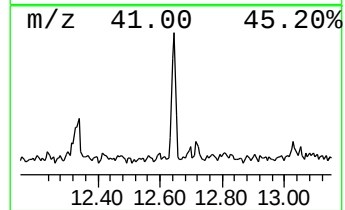
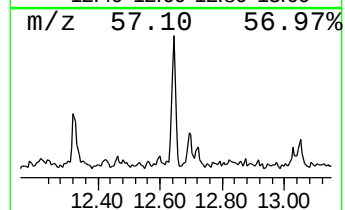
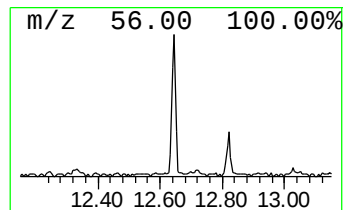
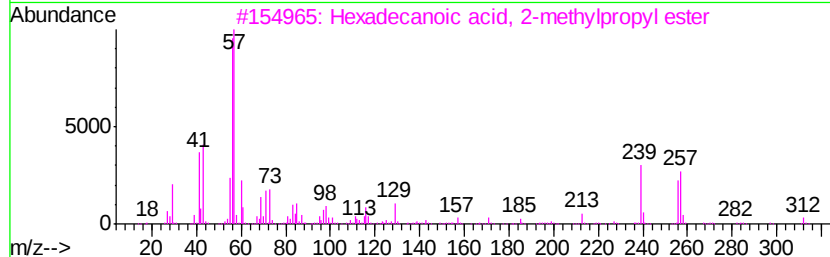
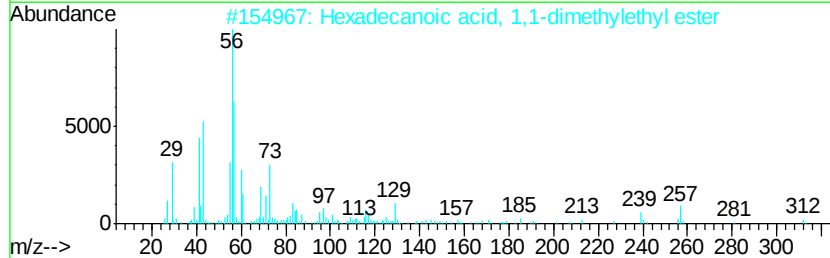
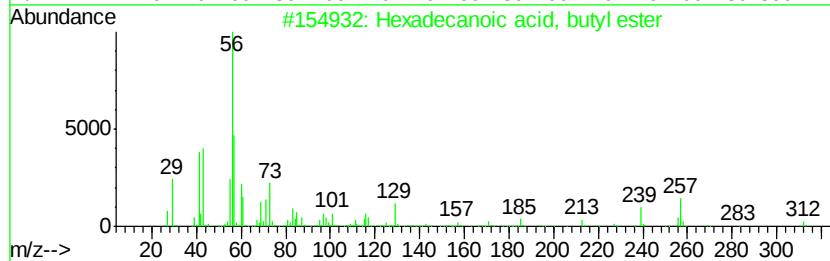
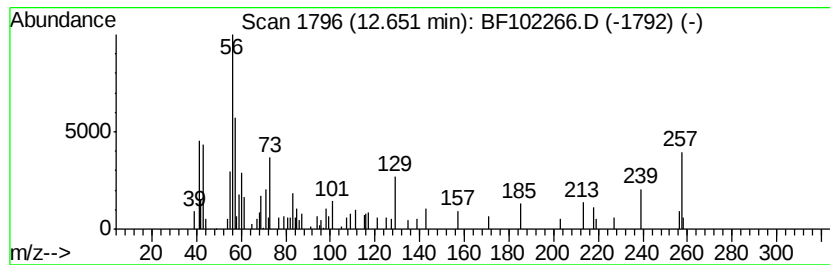
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.70 ng	116334	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	47
4		(n-Butylthio)acetonitrile	129	C6H11NS	071037-08-6	38
5		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35



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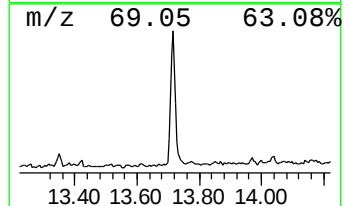
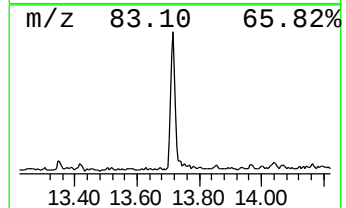
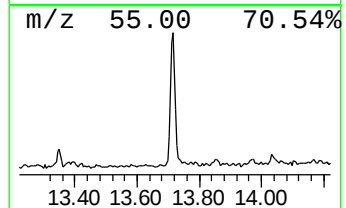
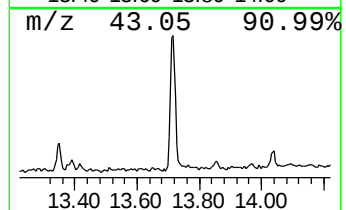
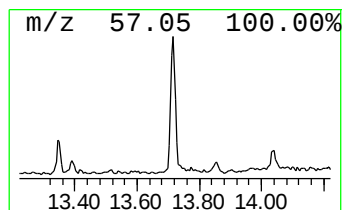
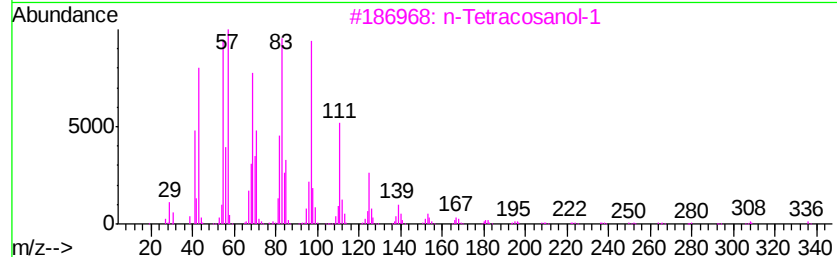
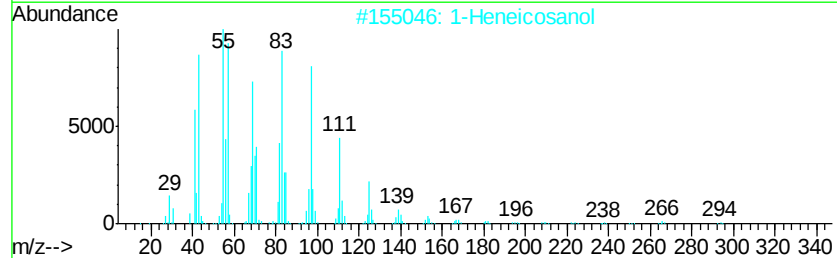
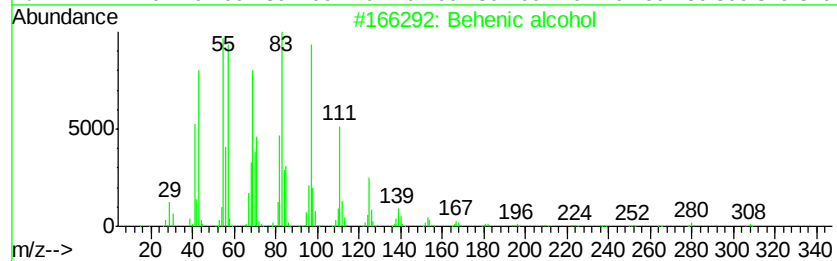
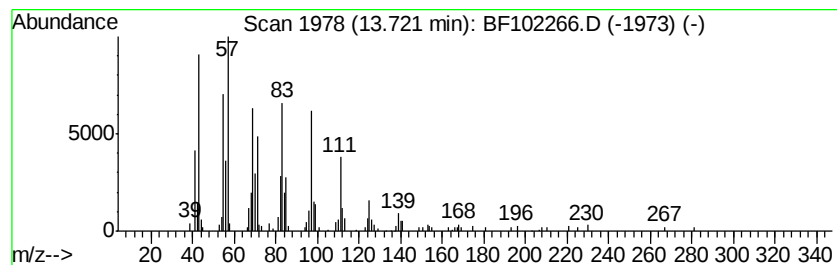
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ClientSampleId :
SB-39-4.0-4.5

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.72	8.32 ng	359005	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	94
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102266.D
Acq On : 20 Jan 2018 15:26
Operator : SJ/JU
Sample : J1115-19
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-39-4.0-4.5

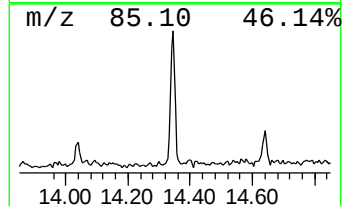
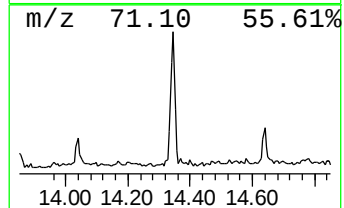
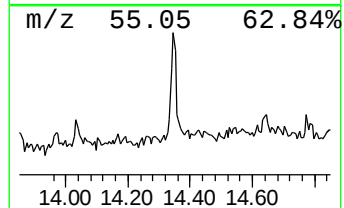
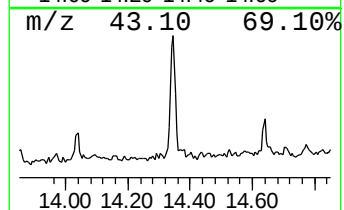
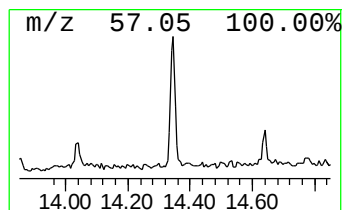
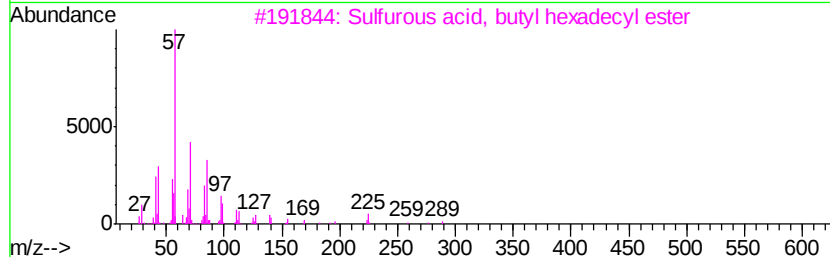
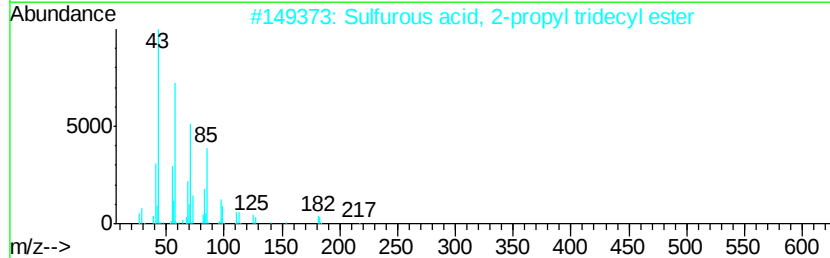
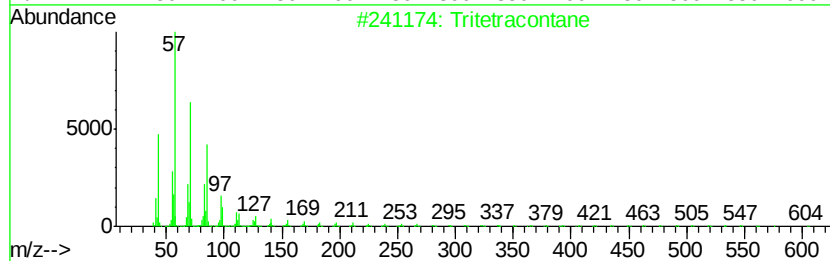
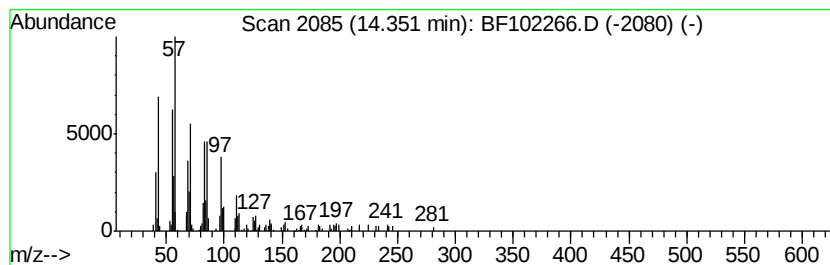
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Tritetracontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	3.73 ng	160701	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tritetracontane	605	C43H88	007098-21-7	91
2		Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	91
3		Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	91
4		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	83
5		10-Methylnonadecane	282	C20H42	056862-62-5	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102266.D
Acq On : 20 Jan 2018 15:26
Operator : SJ/JU
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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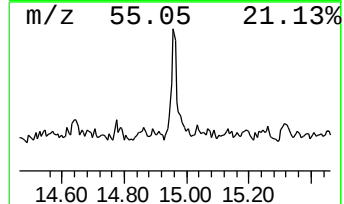
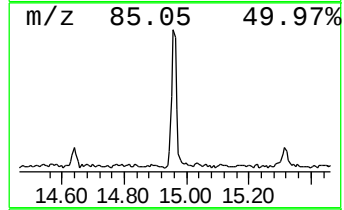
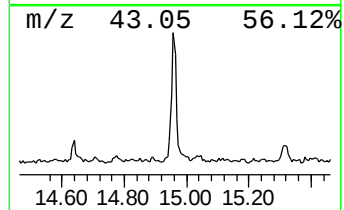
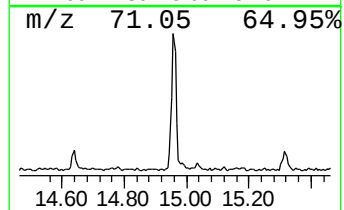
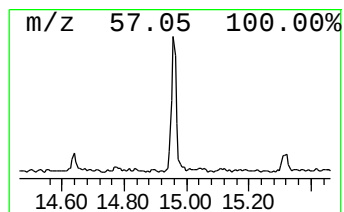
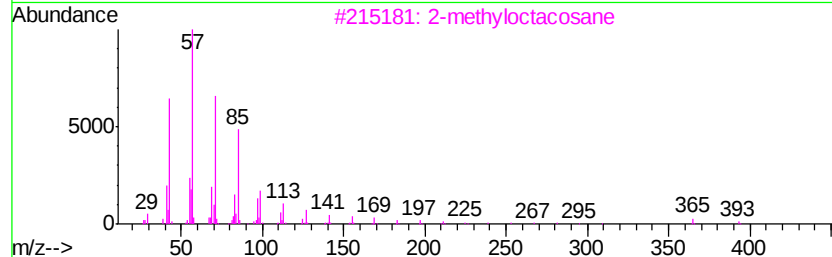
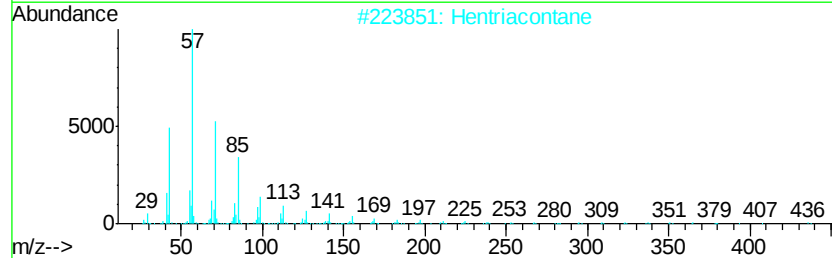
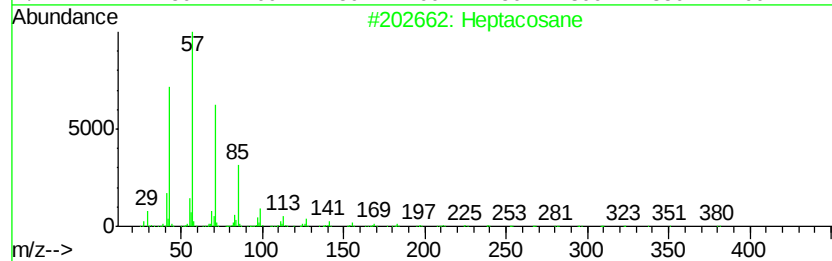
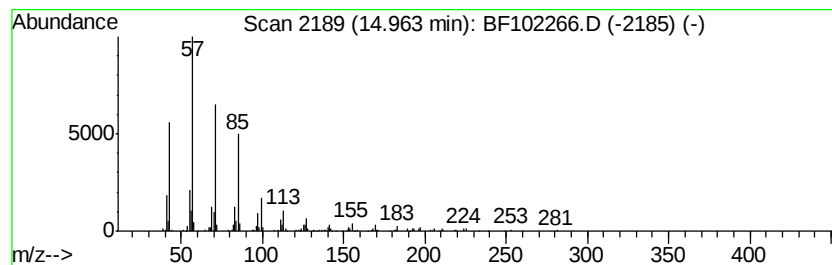
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	6.34 ng	245456	Perylene-d12	15.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Hentriacontane		437	C31H64	000630-04-6	91
3	2-methyloctacosane		408	C29H60	1000376-72-8	90
4	Nonadecane, 2-methyl-		282	C20H42	001560-86-7	90
5	Tetratetracontane		619	C44H90	007098-22-8	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102266.D
Acq On : 20 Jan 2018 15:26
Operator : SJ/JU
Sample : J1115-19
Misc :
ALS Vial : 16 Sample Multiplier: 1

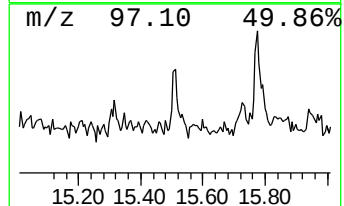
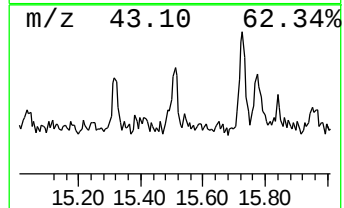
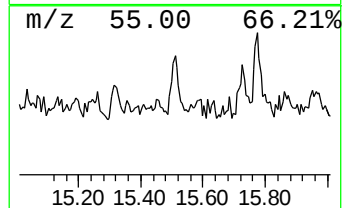
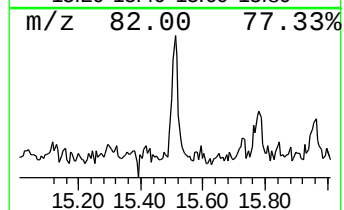
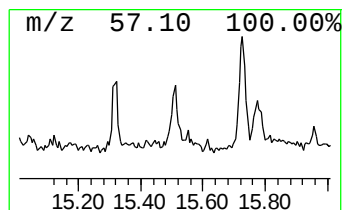
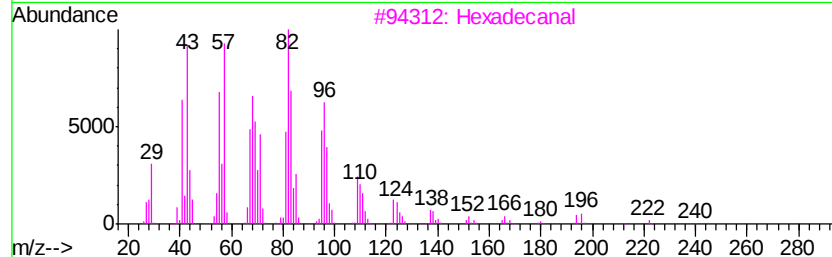
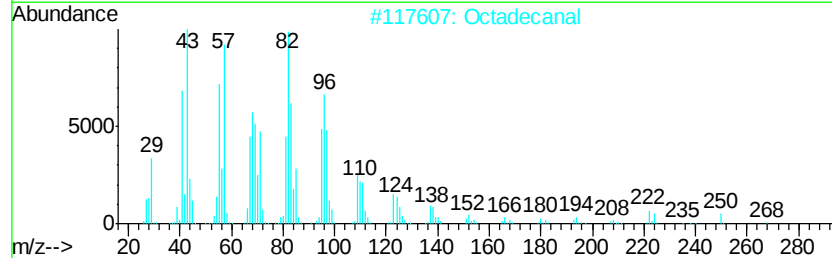
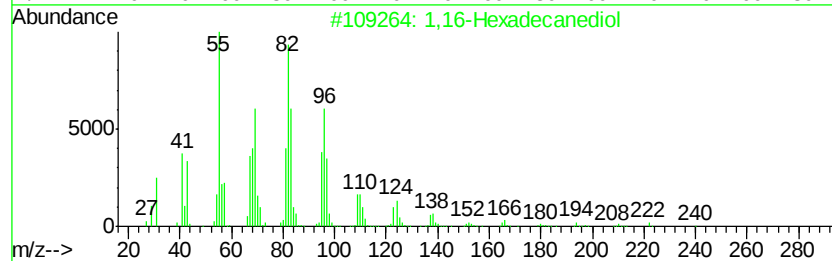
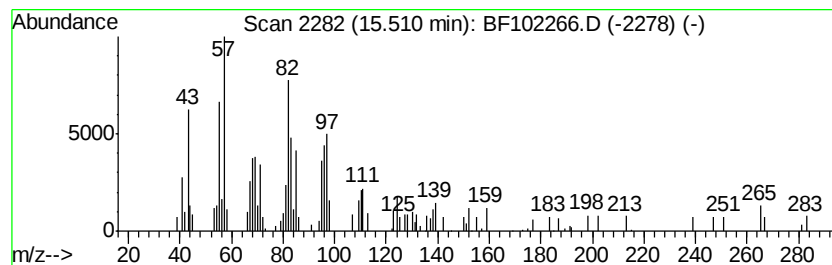
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1,16-Hexadecanediol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.51	2.01 ng	77691	Perylene-d12	15.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	58
2	Octadecanal	268	C18H36O	000638-66-4	58
3	Hexadecanal	240	C16H32O	000629-80-1	58
4	18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	58
5	1,13-Tridecanediol, diacetate	300	C17H32O4	042236-70-4	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
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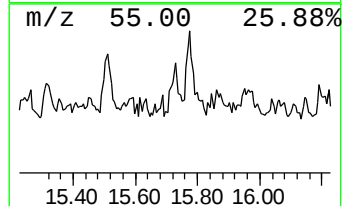
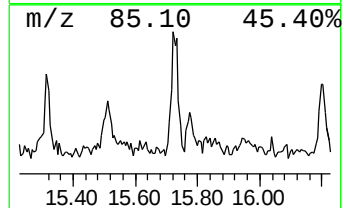
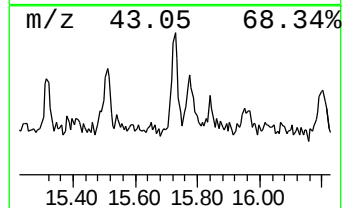
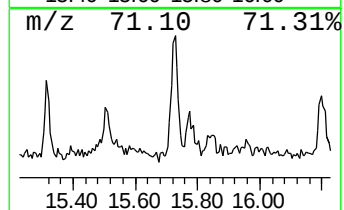
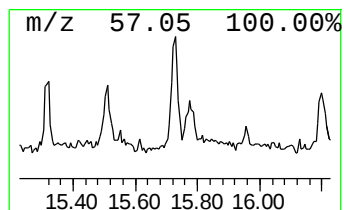
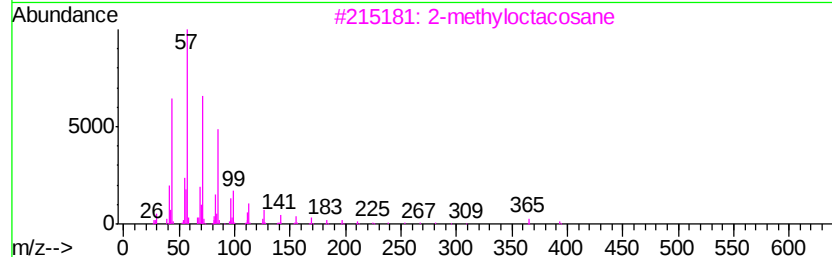
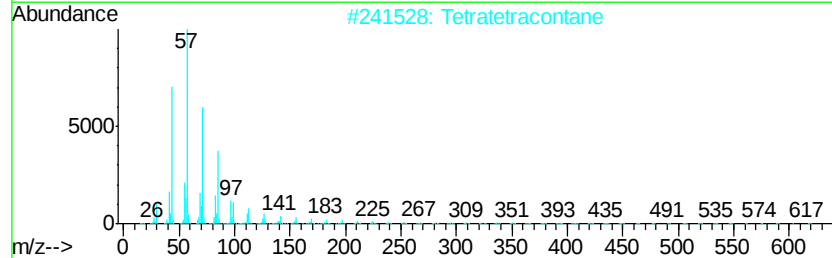
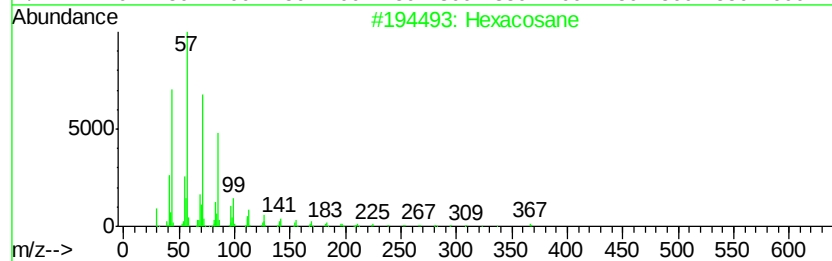
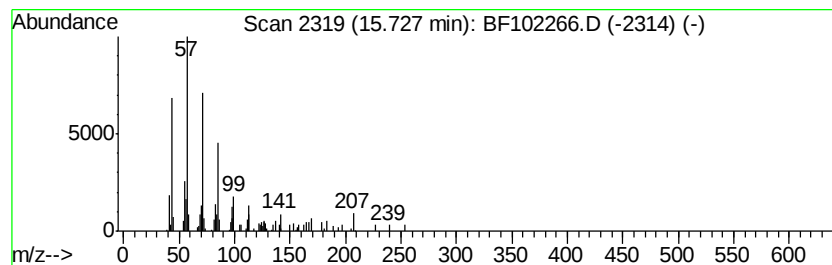
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	2.18 ng	84224	Perylene-d12	15.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	83
2	Tetratetracontane	619 C44H90	007098-22-8	80
3	2-methyloctacosane	408 C29H60	1000376-72-8	80
4	Hentriacontane	437 C31H64	000630-04-6	80
5	Hexadecane	226 C16H34	000544-76-3	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102266.D
Acq On : 20 Jan 2018 15:26
Operator : SJ/JU
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Misc :
ALS Vial : 16 Sample Multiplier: 1

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ClientSampleId :
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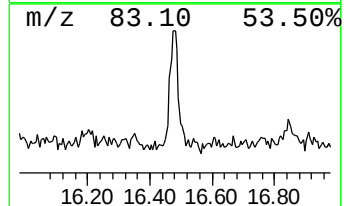
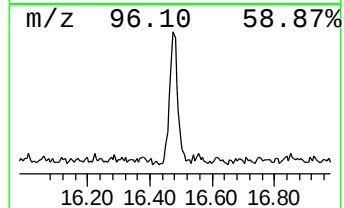
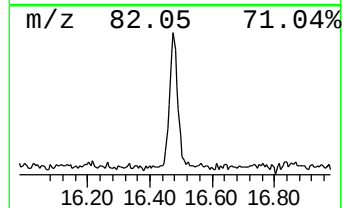
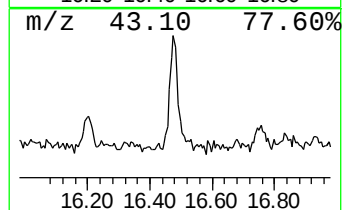
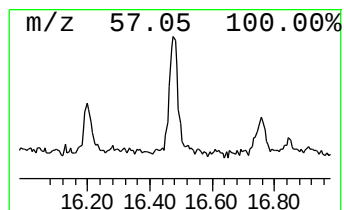
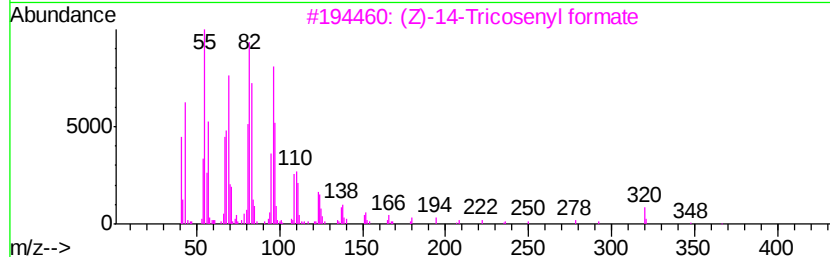
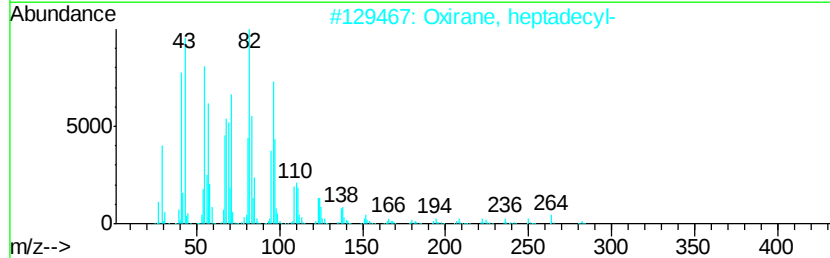
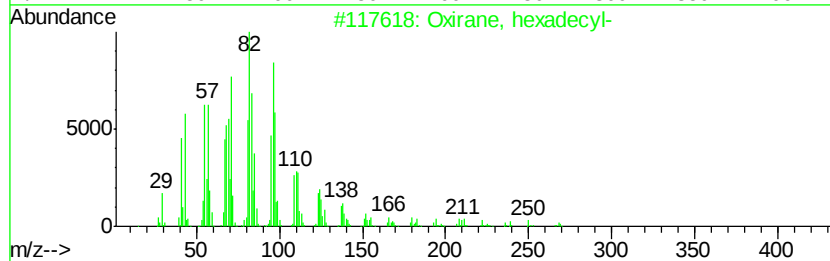
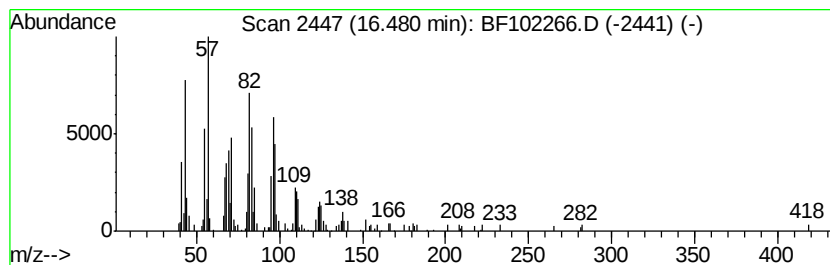
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Oxirane, hexadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.48	5.41 ng	209255	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	95
2		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3		(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	83
4		Octadecanal	268	C18H36O	000638-66-4	74
5		Dodecane, 5-cyclohexyl-	252	C18H36	013151-85-4	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102266.D
Acq On : 20 Jan 2018 15:26
Operator : SJ/JU
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Misc :
ALS Vial : 16 Sample Multiplier: 1

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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	5.8 ng		267778	1	6.72	916068	20.0
unknown6.49	6.49	78.0 ng		3571410	1	6.72	916068	20.0
Hexadecane	10.19	2.2 ng		129172	3	9.75	1164070	20.0
Sulfurous acid, 2...	10.66	2.9 ng		137007	4	11.24	950704	20.0
Hexadecanoic acid...	12.65	2.7 ng		116334	5	13.87	862524	20.0
Behenic alcohol	13.72	8.3 ng		359005	5	13.87	862524	20.0
Tritetracontane	14.35	3.7 ng		160701	5	13.87	862524	20.0
Heptacosane	14.96	6.3 ng		245456	6	15.29	773705	20.0
1,16-Hexadecanediol	15.51	2.0 ng		77691	6	15.29	773705	20.0
Hexacosane	15.73	2.2 ng		84224	6	15.29	773705	20.0
Oxirane, hexadecyl-	16.48	5.4 ng		209255	6	15.29	773705	20.0